# Electronic Structure and Properties of Ultrabright Silicon Nanocrystals

## Motivation

Si nanocrystals in the range of sizes 1-3nm with few tens to hundreds of atoms exhibit **unique optical properties** such as ultrabright luminescence and nonlinear optical effects.

They are easy to prepare, stabilized by hydrogen saturation of the surface atoms, and their properties can be tuned by approapriate doping.

**Goals:** predict the atomic structures, optical properties and change in behaviour upon doping.

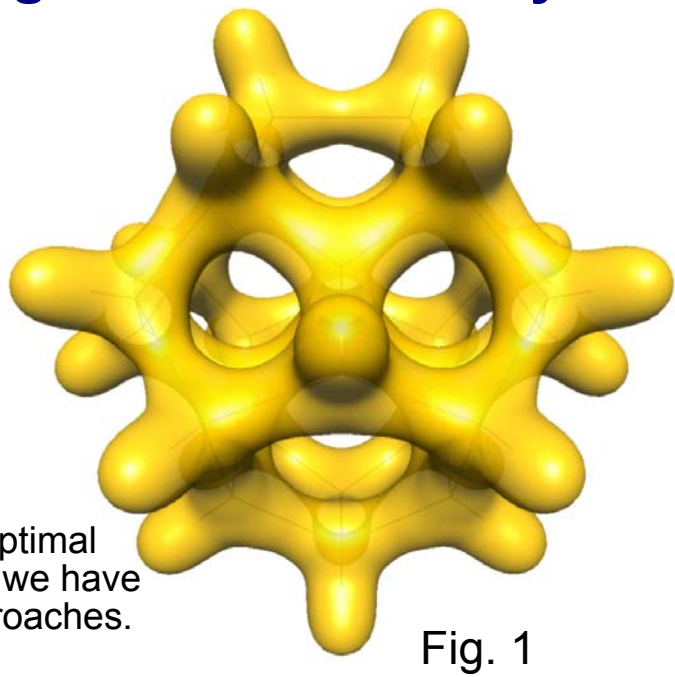
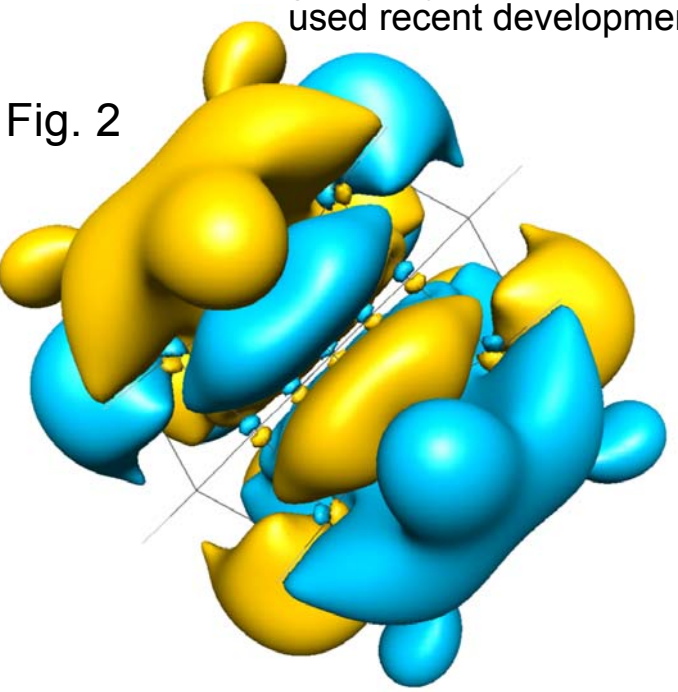


Fig. 1

## Methods

We have used **Density Functional** methods to perform optimal geometry searches. For high accuracy energy differences we have used recent developments in **Quantum Monte Carlo** approaches.

Fig. 2



## Results

**Developed structural proptotypes for various sizes,** eg, in **Fig. 1** is a plot of valence electron density of $Si_{29}H_{24}$, a prototype of the 1nm nanocrystal which, upon excitation, emits blue light.

**Elucidation of the absorption-emission mechanism (Stokes shift):** using a combination of methods we have found that the optical excitons are distributed across the whole nanocrystal (in **Fig. 2** is an isosurface plot of the one-particle excited state) and cause little structural change, contrary to the previous conjectures.

**Prediction of changes of optical properties upon doping** by -NH3, -CH2, and a number of other dopants – confirmed by experiments.

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